# Chemical Sciences and Engineering Aspen LIMS

Customization

## What's New?

Maura Wilhelm

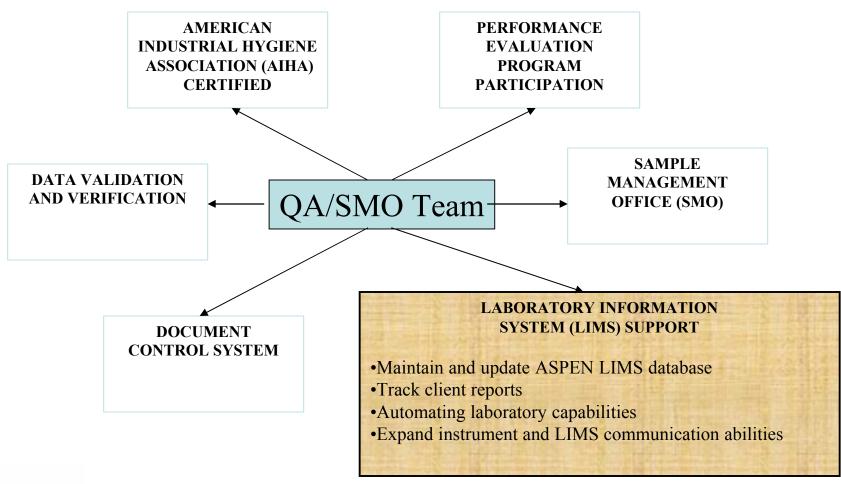
Aspen LIMS Database Administrator





#### UNCLASSIFIED

# Chemistry Division Chemical Sciences and Engineering Group (C-CSE) Quality Assurance/Sample Management Team

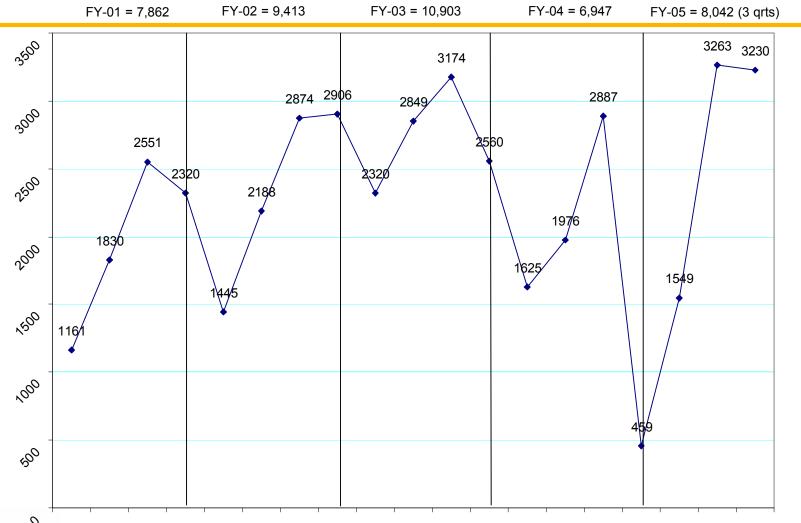






#### UNCLASSIFIED

#### Samples Analyzed and Reported in Aspen by Fiscal Year







## Sample Processing through LIMS Sample Login

Samples collected in field by Health, Safety, and Radiation Protection Industrial Hygienists Samples Received by Sample Management Office personnel



## Aspen Enterprise

Laboratory Information Management System



Samples logged into Laboratory Information Management System (LIMS)

Sample Delivery Package number is assigned in Aspen

Login Sam	ples 10/31/02 14:27 100603
Lab Sample #:	02103105-001 From Schedule:
Ref. ID:	IH Be, Pb, & U Priority: Use Business Days:   ✓
Sample Type:	Filters, Swipe
Customer Sample ID:	LIMS V6 test A Screening Data:
ClientID:	MTW Maura, T. Wilhelm Note: Fifter Swipes for Be, Fb, & U Analysis
Program Code :	00000000000 ID/Work Card #:
Reference Library	Test Group(s) Assigned to Sample:
•	TestGroupID: TestGroup Name: Lab Section: SortNo: Assoc:
Test Group Library	
	<u>E</u> dit Group Order
->∆dd Tast Group->	<u>Modify Tests</u>
Preyiew Tests in Group	Record: I
New Sample	Beplicate Sample Dejete Sample Subcontractors Print SDG Documents

## Sample Processing through LIMS Prep Batch Creation

Digestion Analyst accepts custody of samples from SMO personnel

Analyst completes digestion process in digestion lab

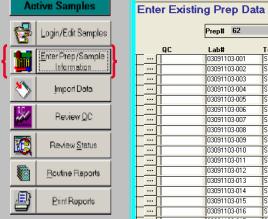
Print Digestion Log Print Auto Sampler Report Back



### Aspen Enterprise

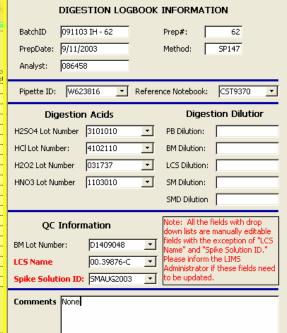
Laboratory Information Management System

#### Los Alamos National Lab



Prep# 62			Prep Date:	Prep Date: 9/11/2003 Prep		086458			
	QC	Lab#	TestGroup ID:	Container ID:	Prep Method:	SampleID	Digestion Dilution	Prep Date	Selec Dele
انند ۲		03091103-001	SP147	03091103-001-01A	SP147	091003SJS1	10	9/11/2003	
<u> </u>		03091103-002	SP147	03091103-002-01A	SP147	091003SJS2	10	9/11/2003	
		03091103-003	SP147	03091103-003-01A	SP147	091003SJS3	10	9/11/2003	
انند ۲		03091103-004	SP147	03091103-004-01A	SP147	091003SJS4	10	9/11/2003	
<u> </u>		03091103-005	SP147	03091103-005-01A	SP147	091003SJS5	10	9/11/2003	
		03091103-006	SP147	03091103-006-01A	SP147	091003SJS6	10	9/11/2003	
		03091103-007	SP147	03091103-007-01A	SP147	091003SJS7	10	9/11/2003	
		03091103-008	SP147	03091103-008-01A	SP147	091003SJS8	10	9/11/2003	
		03091103-009	SP147	03091103-009-01A	SP147	091003SJS9	10	9/11/2003	
		03091103-010	SP147	03091103-010-01A	SP147	091003SJS10	10	9/11/2003	
انند ۲		03091103-011	SP147	03091103-011-01A	SP147	091003SJS11	10	9/11/2003	
<u> </u>		03091103-012	SP147	03091103-012-01A	SP147	091003SJS12	10	9/11/2003	
		03091103-013	SP147	03091103-013-01A	SP147	091003SJS13	10	9/11/2003	
انند ۲		03091103-014	SP147	03091103-014-01A	SP147	091003SJS14	10	9/11/2003	
<u> </u>		03091103-015	SP147	03091103-015-01A	SP147	091003SJS15	10	9/11/2003	
		03091103-016	SP147	03091103-016-01A	SP147	091003SJS16	10	9/11/2003	
		03091103-017	SP147	03091103-017-01A	SP147	091003SJS17	10	9/11/2003	
<u> </u>		03091103-018	SP147	03091103-018-01A	SP147	091003SJS18	10	9/11/2003	
		03091103-019	SP147	03091103-019-01A	SP147	091003SJS19	10	9/11/2003	
		03091103-020	SP147	03091103-020-01A	SP147	091003SJS20	10	9/11/2003	

Edit Prep Data



Done

**Analyst creates prep batch** 

in Aspen

## Sample Processing through LIMS Batch setup on instrument

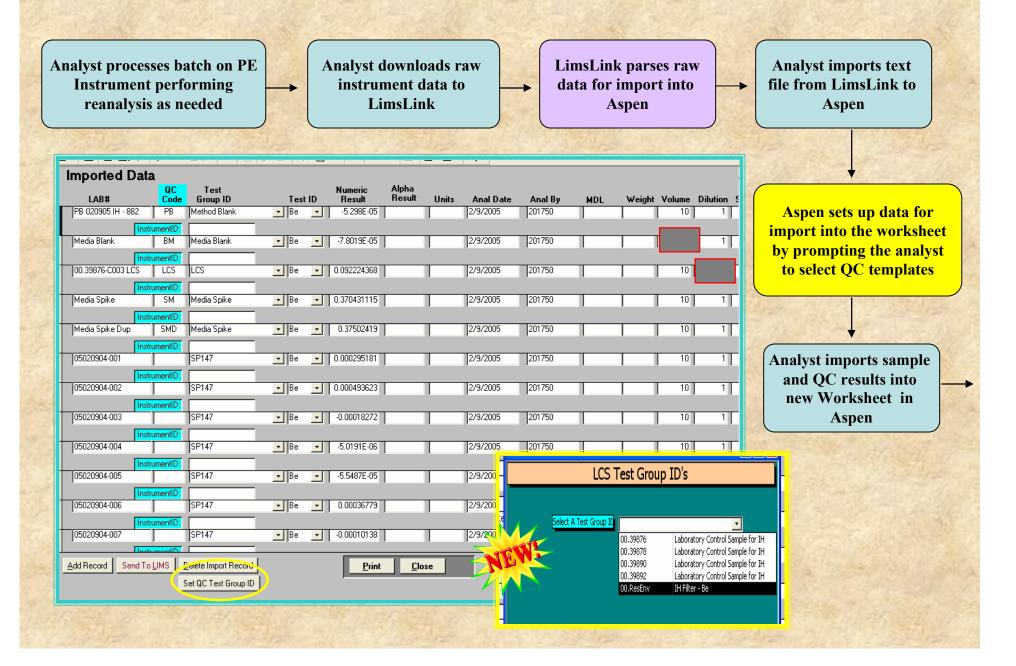
**Analyst creates Digestion Logbook Report and Autosampler Report** 

Analyst loads Autosampler Report into PE WinLab32 Sample Information file

#### DIGESTION LOGBOOK

Batch ID: 093003 IH - 97 Prep#: 97						SMAUG2003			
Prep Date: 9/30/2003 Method: SP147					Spike Received Date: 7/1/2003				
Analyst Straw (101091) Pipette ID/Reference Notebook W623816 / CST9370						Spike Expiration: 7/1/2004			
Digestion	H2SO4 Lot Number: 3101010 H2O2 Lot Number: 31737				Spike Reference Notebook and Page CST9557-57				
Acids:	HCI Lot Number: 4102110 HNC <sub>2</sub> Lot Number: 1103010					Spike Solution Lot # 233454A			
	TICLER Names . 4102110 ELECTRONICE . 1103010								
VESSEL NUMBER	COMMENTS	SDG	SAMPLE INFO	DIGESTION VOLUME	SAMPLE MATRIX	ANALYTE	DUE DATE		
1			PB 093003 IH - 97	10					
2	Lot Number * D1409048		FILTER BLANK BM	10					
3	Lot Number 222820		00.39876-D (TA-59) LCS	10					
4	100 uL		FILTER SPIKE SM	10					
5	100uL		FILTER SPIKE SMD	10					
6		03092902-001		10	Filters, Swipe	Be. Pb. U	10/2/2003		
7		03092902-002		10	Filters, Swipe	Be, Pb, U	10/2/2003		
8		03092902-003		10	Filters, Swipe	Be. Pb. U	10/2/2003		
9		03092902-004		10	Filters, Swipe	Be, Pb, U	10/2/2003		
10		03092902-005		10	Filters, Swipe	Be, Pb, U	10/2/2003		
11		03092902-005		10	Filters, Swipe	Be, Pb, U	10/2/2003		
12		03092902-007		10	Filters, Swipe	Be, Pb, U	10/2/2003		
13		03092902-008		10	Filters, Swipe	Be, Pb, U	10/2/2003		
14		03092902-009	16817	10	Filters, Swipe	Be, Pb, U	10/2/2003		
15		03092902-010		10	Filters, Swipe	Be, Pb, U	10/2/2003		
16		03092902-011		10.5	Filters, Swipe	Be, Pb, U	10/2/2003		
17		03092902-012		10	Filters, Swipe	Be, Pb, U	10/2/2003		
18		03092902-013	, ,	10	Filters, Swipe	Be, Pb, U	10/2/2003		
19		03092902-014		10	Filters, Swipe	Be. Pb. U	10/2/2003		
20		03092902-015		10	Filters, Swipe	Be. Pb. U	10/2/2003		
21		03092902-016		10	Filters, Swipe	Be. Pb. U	10/2/2003		
22		03092902-017		10	Filters, Swine	Be. Pb. U	10/2/2003		
23		03092902-018		10	Filters, Swipe	Be. Pb. U	10/2/2003		
24		00092902-019		10	Filters, Swipe	Be. Pb. U	10/2/2003		
25		03092902-020		10	Filters, Swipe	Be. Pb. U	10/2/2003		
	*Filter Spike and Filter Spike Dup are t	the same lot number as th	e Filter Blank.		•				

Sample Analysis and Import



Analysis Results Import to Worksheet and QC Flagging

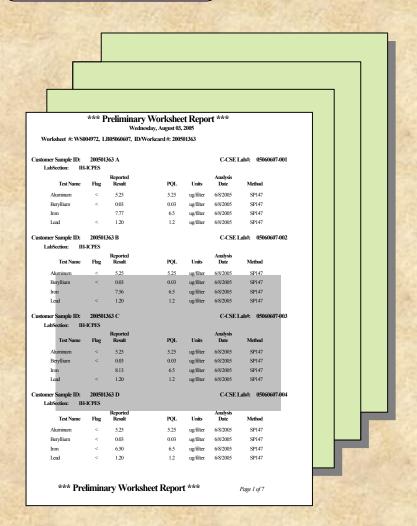
**Analyst imports results Aspen calculates Reported** automatically via Aspen's Results for Samples based on **Import Process into new** raw data imported from Worksheet instrument. 99 - Inorganic 01 - Radchem Enter TEST Results QC Prefix: 03 WS#: WS005122 Lab Section: QC Lab# Customer Sample ID Test Group ID Test 05072903-001 072605RBS01 0.000224105 Comments: 05072903-002 072605RBS02 SP147 10 0.0002849466 CalcResult 0.0028494665 CalcMDL 0.03 **Aspen calculates Reported** 05072903-003 072605RBS03 10 ug/filter **Results for OC and sets** 0103848519 CalcMDL 0.03 flags based on QC template 05072903-004 072605RBS04 SP147 4.165826E-05 ug/filter 10 Comments: CalcResult 0.0004165826 CalcMDL 0.03 parameters. 05072903-005 072605RBS05 SP147 0.003 10 CalcResult 0.0008070057 CalcMDL 0.03 Comments: 05072903-006 072605RBS06 SP147 10 ug/filter CalcResult 0.0018397290 CalcMDL 0.03 Comments: 05072903-007 072605RBS07 SP147 8.209995E-05 ug/filter All QC 05072903-008 072605RBS08 QC Test QC NT True/Added: Group ID QC Test ID 0.0062568389 CalcMDL 0.03 Instrument QC Lab# 00.36898 0.09 **-**0.0 vledia Blank 05072903-009 072605RBS10 24135 Sigma : CalcResult 0.001534803 CalcMDL 0.03 Comments: Instrument Media Spike SMJUN2005-5: Be 0.0 RPD Flag LIMS#: 24136 Sigma : %R Flag 10 Relative P<u>r</u>e Data Trends View QC Media Spike Dup SMDJUN2005 Be 0.3254004564 ▼ 0.0 Relative User Ext. <u>Print</u> <u>B</u>ack RPD Flag 10 Relative ▼ 0.0 00.39756 24138 Sigma Microsoft Access

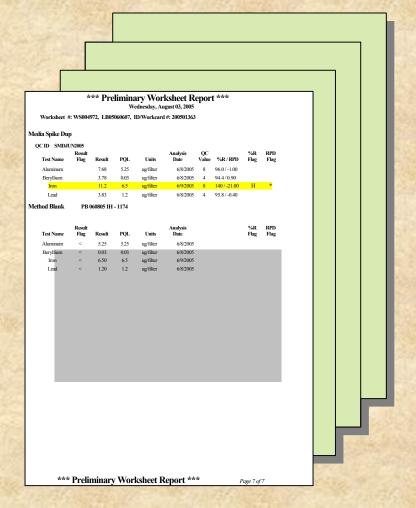
**Preliminary Reporting in Aspen** 

Analyst compiles Data Package consisting of all documents and reports related to Sample

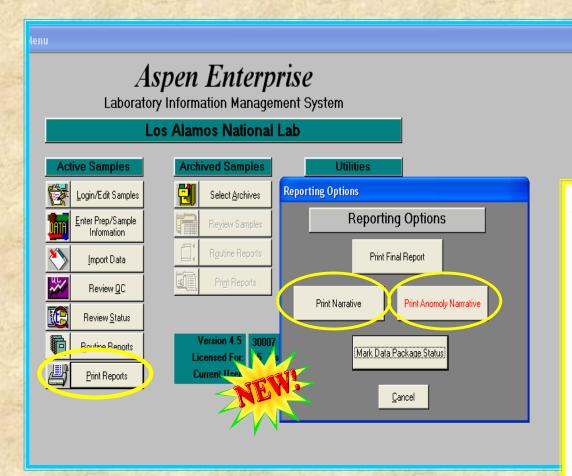
Data Package is sent to peer review

Analyst generates a Preliminary Report which is Emailed to Customer





Narrative Reporting in Aspen





ToMS: Kay Kams, HSR-8, MS C925 FromMS: Chris Brink, C-CSE, MS K484 PhoneFrax: 667-0152 / 665-5982 Symbol: C-CSE, IH (68072601 Date: August 4, 2005

#### ----

Subject: Analytical Results - SDG#: 05072601 ID/Workcard#: 200501147

This analytical request was logged on 7/26/2005 and included 16 Swipe Filters to be analyzed for Beryllium, Lead, & Utanium. All samples received by this laboratory on 7/26/2005 were in acceptable condition. Each sample was analyzed using analytical method SP147. Analysis was completed on 7/27/2005. My records indicate a preliminary report was electronically mailed to you on 7/27/2005. Results are included in Section 2 of this report.

#### QC.

Two Media Spikes, two Blank QC samples and one Laboratory Control Sample (LCS) were analyzed concurrently with the field samples. All QC results were within acceptable ranges.

#### Comments

The analytical results contained in this report relate only to the items tested, and do not have any blank corrections (e.g., field blanks or method blanks are not subtracted from the results).

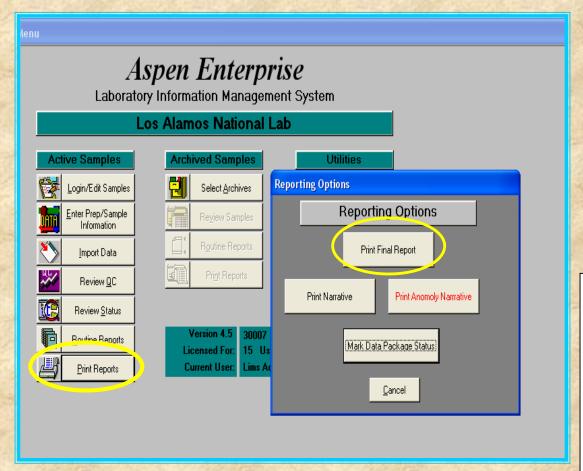
\*\*\*Digestion Comments (directly from Aspen Digestion Log)

#### None

No anomalies were observed with your samples. If you have any questions regarding this data, please give me a call.

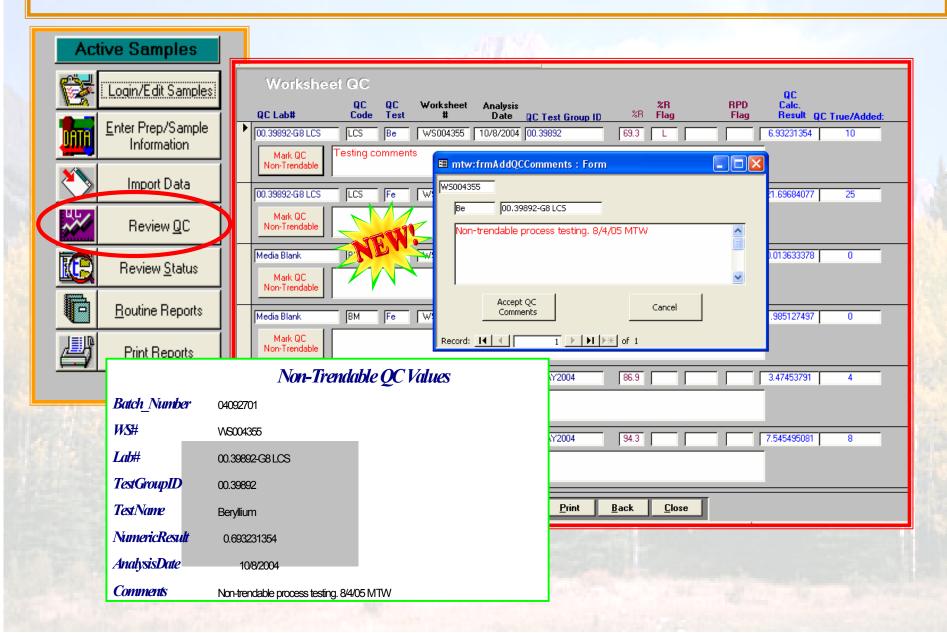
Cy: IH File

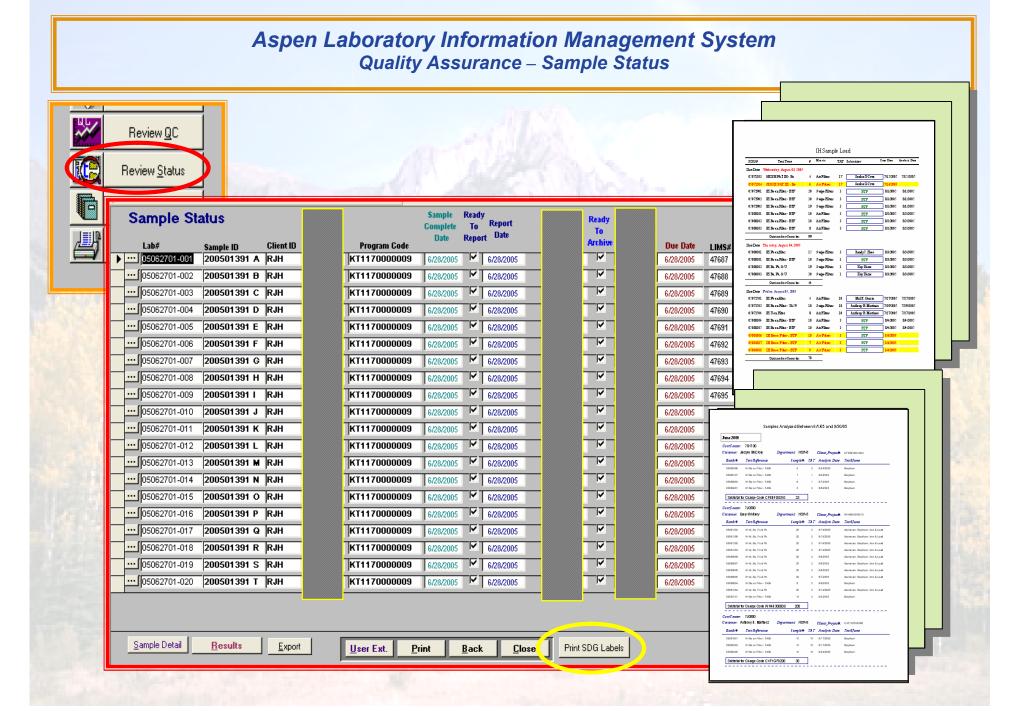
Final Reporting in Aspen



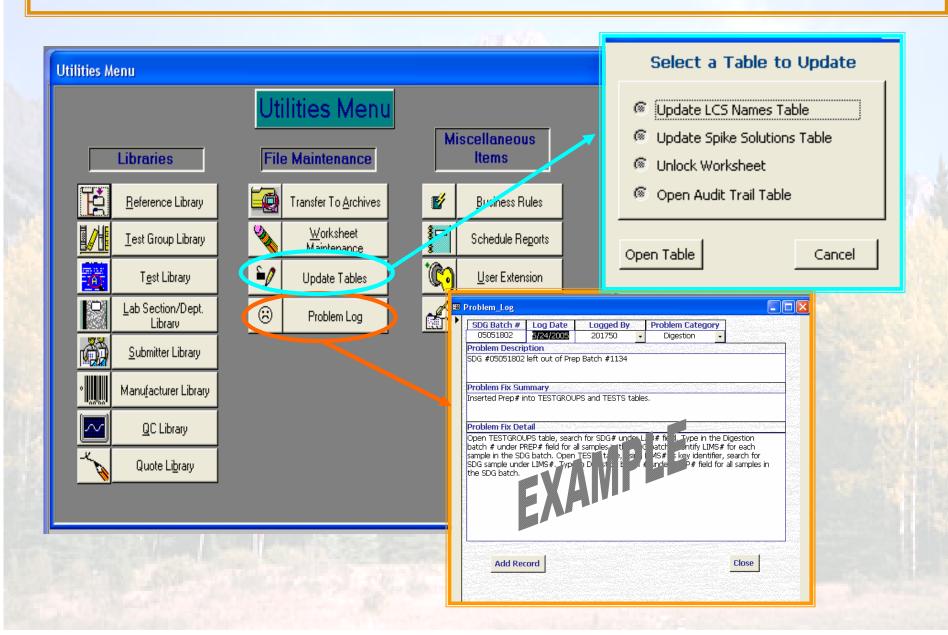


#### Aspen Laboratory Information Management System Quality Assurance – Non-Trendable QC module





## Aspen Laboratory Information Management System Utilities Menu



## Aspen Laboratory Information Management System Database Customizations

#### **Active Samples**



Login/Edit Samples



Enter Prep/Sample Information



Import Data



Review QC



Review Status



Routine Reports



Print Reports

**Amended Login Report** 

Prep Batch Creation and Modification; Dilution Flagging; Autosampler Report

QC Template Assignment; Digestion Dilution Transfer

Non-Trendable Module; Auto-import of QC data

**Data Package Tracking** 

**IH Sample Load Report** 

**Online Narrative; Merged Anomaly Narrative** 

#### What's in the works?

- Run-time analysis flagging program to interface with Perkin-Elmer instruments
- MiniTab Trending software implementation:
  - Automatic QC Trending Charts available for each data packet
  - QC Trending Charts for each month updated automatically
- Interfacing LIMS with various Radiological Instrumentation
- Sharepoint Interface
  - Sample login to Aspen initiated by HSR Industrial Hygienists
  - Interface directly with Customer databases



